

JET-COOLED INFRARED LASER SPECTROSCOPY IN THE UMBRELLA ν_2 VIBRATION REGION OF NH_3 : IMPROVING THE POTENTIAL ENERGY SURFACE MODEL OF THE $\text{NH}_3 - \text{Ar}$ VAN DER WAALS COMPLEX

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Taking advantage of our sensitive laser spectrometer coupled to a pulsed slit jet^b we recorded near the ν_2 vibration a series of rovibrational transitions of the $\text{NH}_3 - \text{Ar}$ van der Waals (vdW) complex. These transitions involve in the ground vibrational state several internal rotor states corresponding to the ortho- NH_3 and para- NH_3 spin modifications of the complex. They are labeled by $\Sigma_a(j,k)$, $\Sigma_s(j,k)$, $\Pi_a(j,k)$ and $\Pi_s(j,k)$ where $\Sigma(K=0)$ and $\Pi(K=1)$ indicate the projection K of the total rotational angular momentum J on the vdW axis, the superscripts s and a designate a symmetric or antisymmetric NH_3 inversion wave function, and j , k quantum numbers indicate the correlation between the internal-rotor state of the complex and the j , k rotational state of the free NH_3 monomer. Five bands have been identified, only one of which was partly observed before^c. They include transitions starting from the $\Sigma_a(j=0 \text{ or } j=1)$ state without any internal angular momentum, consequently they can be assigned from the band contour of a linear-molecule-like $K=0$, $\Delta J=1$ transition. The energies and splittings of the rovibrational levels of the $\nu_2 = 1 \leftarrow 0$ spectrum derived from the analysis of the Π_s , $\Sigma_s(j=1) \leftarrow \Sigma_a(j=0)$, $k=0$ bands and mostly of the Σ_s , Π_s and $\Sigma_a(j=1) \leftarrow \Sigma_a(j=1)$, $k=1$ bands bring relevant information about the ν_2 dependence of the $\text{NH}_3 - \text{Ar}$ interaction, the rovibrational dynamics of the $\text{NH}_3 - \text{Ar}$ complex and provide a sensitive test of a recently developed 4D potential energy surface that includes explicitly its dependence on the umbrella motion^d.

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